

# On the temperature dependence of the superconducting gap in high- $T_c$ cuprates

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(Dated: 17 January, 2005)

It is proposed that (i) the temperature dependence of the superconducting gap  $\Delta(T)$  in high- $T_c$  cuprates can be predicted just from the knowledge of  $\Delta(0)$  and the critical temperature  $T_c$ ; and, in particular, (ii)  $\Delta(0)/T_c > 4$  implies that  $\Delta(T_c) \neq 0$ , while  $\Delta(0)/T_c \leq 4$  corresponds to  $\Delta(T_c) = 0$ . A number of tunneling experiments appear to support the above proposition, and, furthermore, show reasonable quantitative agreement with a model based on the two-dimensional stripe hypothesis.

PACS numbers: 74.50.+r, 74.72.-h, 74.20.Mn, 74.25.Jb

In conventional superconductors, the phenomenology of the superconducting (SC) energy gap closely follows that of the model of Bardeen, Cooper and Schrieffer (BCS)[1]. Namely: (i) Below the SC transition temperature ( $T_c$ ), there are no one particle excitations within the SC gap  $\Delta(T)$ , where  $T$  is the temperature; (ii) At the gap boundaries  $\pm\Delta(T)$ , there are symmetric SC peaks; (iii) The ratio  $\Delta(0)/T_c$  is close to 1.76; (iv)  $\Delta(T_c) = 0$ . In contrast, the tunneling studies of high- $T_c$  cuprates show that: (i) The density of states within the SC gap is not zero; (ii) The SC peaks are frequently asymmetric; (iii) The ratio  $\Delta(0)/T_c$  is significantly larger than 1.76 and not universal; (iv) There are indications that, in some high- $T_c$  compounds,  $\Delta(T_c) \neq 0$ . The above non-universality implies that any BCS-like one-parameter description of the tunneling spectra cannot be adequate for high- $T_c$  cuprates. The complexity of these materials further suggests that their proper microscopic description should contain many parameters. In this work, however, I report a surprising finding that the phenomenology of the SC gap in high- $T_c$  cuprates may be describable by only two parameters.

The present study was originally undertaken to test a simple model proposed in Ref. [2]. The calculations of the tunneling characteristics based on that model require only two input parameters  $\Delta(0)$  and  $T_c$ . The reasonable success of this test, of course, lends credibility to the model, but also, irrespectively of the model, it suggests that, even though the ratio  $\Delta(0)/T_c$  may exhibit a non-universal doping dependence, and, moreover, may be different for different samples of the same material, the measured values of  $\Delta(0)$  and  $T_c$  are sufficient to predict the entire evolution of  $\Delta(T)$ . Of particular interest is the following model-based rule:

$$\begin{aligned} \Delta(0)/T_c > 4 &\Leftrightarrow \Delta(T_c) \neq 0 / \text{asymmetric SC peaks;} \\ \Delta(0)/T_c \leq 4 &\Leftrightarrow \Delta(T_c) = 0 / \text{symmetric SC peaks.} \end{aligned} \quad (1)$$

It was the surprisingly good agreement of the symmetry/asymmetry part of this rule with many experiments[2], that prompted me to test the model pre-

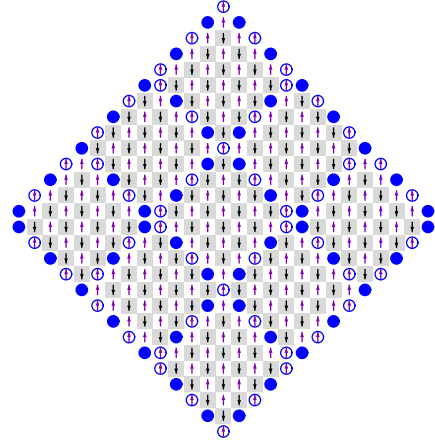


FIG. 1: 2D configuration of diagonal stripes (a cartoon).

dictions for the shape of the  $\Delta(T)$ -curve.

The model of Ref. [2] is based on the hypothesis that a two-dimensional (2D) arrangement of stripes shown in Fig. 1 exists in the  $\text{CuO}_2$  planes of high- $T_c$  cuprates. In such a superstructure, there exist hole states localized either inside the stripes (b-states) or in the antiferromagnetic (AF) domains between the stripes (a-states). Due to the small size of the AF domains and stripe elements ( $20 - 30\text{\AA}$ ), the energy levels within each unit should be broadly spaced (estimated[2] as 40 meV). The model proceeds by assuming the existence of only one low-energy a-state per AF domain and two low-energy b-states per stripe element. As argued in Ref. [2], a promising choice for the model Hamiltonian is

$$\begin{aligned} \mathcal{H} = & \varepsilon_a \sum_i a_i^\dagger a_i + \varepsilon_b \sum_{i,j(i),\sigma}^{n_i=1} b_{ij,\sigma}^\dagger b_{ij,\sigma} \\ & + g \sum_{i,j(i)}^{n_i=1} (b_{ij,+}^\dagger b_{ij,-}^\dagger a_i a_j + \text{h. c.}), \end{aligned} \quad (2)$$

where index  $i$  or  $j$  labels AF domains;  $j(i)$  implies, that

the  $j$ th AF domain is the nearest neighbor of the  $i$ th domain;  $a_i$  is the annihilation operator of a hole inside the  $i$ th AF domain;  $b_{ij,\sigma}$  is the annihilation operator of a hole inside the stripe element separating the  $i$ th and the  $j$ th AF domains;  $\sigma$  is the spin index, which can have two values “+” or “-”;  $\varepsilon_a$  and  $\varepsilon_b$  are position-independent on-site energies for a- and b-states, respectively, counted from the chemical potential; and, finally,  $g$  is the coupling constant. The spins of a-states are tracked by index  $\eta_i$ , which alternates between 1 or  $-1$  thus tracing the sign of the AF order parameter in the AF domains. The sum superscript “ $\eta_i = 1$ ” indicates that the summation extends only over the supercells having  $\eta_i = 1$ .

The total energy of such a system as a function of the chemical potential  $\mu$  has at least two minima[2]:  $\mu = \varepsilon_a$  and  $\mu = \varepsilon_b$ , which implies two most promising regimes — Case I:  $\varepsilon_b = 0$ ; and Case II:  $\varepsilon_a = 0$ . The mean-field solution then leads to the density of states described by the following system of equations[2]: in Case I,

$$\varepsilon_A(\mathbf{k}) = \sqrt{\varepsilon_a^2 + \frac{1}{4}g^2(2n_B - 1)^2|V(\mathbf{k})|^2}, \quad (3)$$

$$\varepsilon_B = -\frac{g^2(2n_B - 1)}{64\pi^2} \int_{-\pi}^{\pi} dk_x \int_{-\pi}^{\pi} dk_y \frac{(1 - 2n_A(\mathbf{k})|V(\mathbf{k})|^2}{\varepsilon_A(\mathbf{k})}, \quad (4)$$

and, in Case II,

$$\varepsilon_A(\mathbf{k}) = -\frac{g^2|V(\mathbf{k})|C_a(1 - 2n_B)}{8\varepsilon_B}, \quad (5)$$

$$\varepsilon_B = \sqrt{\varepsilon_b^2 + \frac{1}{16}g^2C_a^2}, \quad (6)$$

where subscripts  $A$  and  $B$  indicate the Bogoliubov quasiparticles associated with a- and b-states, respectively;  $\varepsilon_{A/B}$  and  $n_{A/B}$  are the quasiparticle energies and the occupation numbers, respectively. A-quasiparticles are characterized by well-defined wave vectors  $\mathbf{k}$ . All B-quasiparticles have the same  $\varepsilon_B$ . The expressions for  $n_A(\mathbf{k})$  and  $n_B$ , and for the auxiliary quantities  $C_a$  and  $V(\mathbf{k})$  are:

$$n_A(\mathbf{k}) = \frac{1}{\exp\left(\frac{\varepsilon_A(\mathbf{k})}{T}\right) + 1}, \quad (7)$$

$$n_B = \frac{1}{\exp\left(\frac{\varepsilon_B}{T}\right) + 1}, \quad (8)$$

$$V(\mathbf{k}) = 2 \left[ \cos\left(\frac{k_x + k_y}{2}\right) - i \cos\left(\frac{k_x - k_y}{2}\right) \right], \quad (9)$$

$$C_a = \frac{1}{8\pi^2} \int_{-\pi}^{\pi} dk_x \int_{-\pi}^{\pi} dk_y (2n_A(\mathbf{k}) - 1)|V(\mathbf{k})|. \quad (10)$$

The tunneling spectra of A-states have Van Hove singularities, which, in Case I, are located at

$$\varepsilon_{A0} = \pm \sqrt{\varepsilon_a^2 + g^2(2n_B - 1)^2}. \quad (11)$$

and, in Case II, at

$$\varepsilon_{A0} = \pm \frac{g^2C_a(1 - 2n_B)}{4\varepsilon_B} \quad (12)$$

Three representative zero-temperature tunneling spectra of both A- and B-states can be found in Ref. [2].

In both Cases I and II, the mean-field  $T_c$  can be obtained [2] numerically from the following equation:

$$T_c = \frac{g^2 \left[ \exp\left(\frac{|\varepsilon_a - \varepsilon_b|}{T_c}\right) - 1 \right]}{8|\varepsilon_a - \varepsilon_b| \left[ \exp\left(\frac{|\varepsilon_a - \varepsilon_b|}{T_c}\right) + 1 \right]}. \quad (13)$$

Given the above picture, the basic features of the tunneling phenomenology can be interpreted as follows: (1) The SC peaks at  $\pm\Delta$ , are identified with the Van Hove singularities at  $\pm\varepsilon_{A0}$  in the density of A-states. (2) The density of B-states is assumed to be more difficult to detect due to, perhaps, smaller tunneling elements.

The knowledge of  $\Delta(0)$  and  $T_c$  is thus sufficient to obtain the model parameters  $|\varepsilon_a|$  and  $g$  in Case I [Eqs.(11,13) with  $n_B = 1$ ], and  $|\varepsilon_b|$  and  $g$  in Case II [Eqs.(6,9,10,12,13) with  $n_A(\mathbf{k}) = 1; n_B = 0$ ]. After that,  $\Delta(T)$  can be calculated numerically using Eqs.(3-12) without additional adjustable parameters. Importantly, Cases I and II do not overlap in terms of the ratio  $\Delta(0)/T_c$ : in Case I,  $\Delta(0)/T_c > 4$ , while in Case II,  $\Delta(0)/T_c < 4$ . The entire family of the  $\Delta(T)$ -curves is presented in Fig. 2.

In both Cases I and II,  $|\varepsilon_a - \varepsilon_b|$  is a measure of the pseudogap (see Sec.V of Ref. [2]). This pseudogap is a real feature in the normal density of states (as, e.g., in the proposal of Ref.[3]), i.e., it is not associated with the SC fluctuations above  $T_c$ . This feature is a generic consequence of the nanoscale phase separation — two different kinds of real space regions (stripes and AF domains) imply two different energies associated with them. The model pseudogap equals zero only in the critical case,  $\varepsilon_a = \varepsilon_b$ , which, as argued in Ref.[2], may correspond to the doping concentration 0.19. The model has two different SC energy gaps:  $\varepsilon_{A0}$  for A-states and  $\varepsilon_B$  for B-states. In Case I,  $\varepsilon_B$  turns to zero at  $T = T_c$ , while  $\varepsilon_{A0}$  becomes equal to the pseudogap  $|\varepsilon_a - \varepsilon_b|$ . In Case II, the situation at  $T = T_c$  is opposite:  $\varepsilon_{A0} = 0$ , while  $\varepsilon_B = |\varepsilon_a - \varepsilon_b|$ . Thus the difference between the two model regimes is not qualitative but only quantitative. However, since, by assumption, the observable SC peaks represent only A-states, the phenomenology of the SC gap appears to be qualitatively different in the two regimes.

In Fig. 3, I compare the theoretical predictions with the results of the break junction (BJ)[4, 5, 6] and the

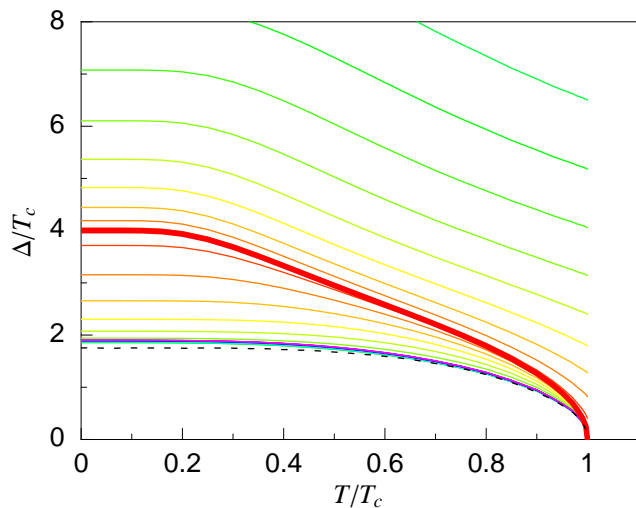


FIG. 2: (Color online) Family of theoretical curves for the temperature dependence of the superconducting gap. Thick line corresponds to the critical ratio  $\Delta(0)/T_c = 4$ . Solid lines above the thick line describe Case I, and below the thick line Case II. The dashed line represents the BCS result.

interlayer tunneling (ILT)[7, 8, 9, 10, 11, 12] experiments. The ILT technique gives better energy resolution and comes closer to measuring the true intrinsic density of states in the bulk of cuprates, but, at the same time, it generates significant overheating of the sample. In order to avoid this problem, the authors of Refs.[7, 8, 12] have used a short-pulse method, which, however, comes at a cost of somewhat lower energy resolution [Figs. 3(c-g) and (q-s)]. Alternatively, the authors of Refs.[9, 10, 11, 13] [Figs. 3(h-n) and (t)] have perfected the “conventional” ILT technique by manufacturing sufficiently small *mesas* and thus reducing the overheating. In the latter case, the experimental data points reflect the ambient temperature of experiment. The question, however, remains concerning the true value of the temperature of the *mesas*[14, 15]. Theoretical and experimental estimates made in Refs.[13, 16, 17], have indicated possible significant overheating, but there is still a chance that, at least in the underdoped Bi-2212, the temperature was not too much distorted at the voltage biases probing the SC peaks.

Most of the theoretical curves shown in Fig. 3 agree with the experimental data within the limits of [sometimes, large] uncertainty associated with the broadening of the SC peaks (see the original references). The data points in Fig. 3 are obtained from the peak-to-peak separation in the experimental tunneling spectra. Usually, the peak broadening shifts the peak maximum towards higher energies. If this effect is undone by extracting the “bare” values of  $\Delta$ , then the experimental points in Figs. 3(a-g,o,q-s) would appear significantly closer to the theoretical curves. This is a consequence of the fact that

the SC peaks are broader at higher temperatures. The magnitude of the above correction can be judged on the basis of the estimates of bare  $\Delta$  made in Ref.[5] and presented in Fig. 3(a,b). [Note: the widths of the SC peaks corresponding to Figs. 3(a,b) are comparable or smaller than those corresponding to Figs. 3(d-g,o-s).]

The agreement between the theory and the experiment is typically better, whenever the SC peaks are sharper. This is, particularly, true for the “pulsed” ILT experiments (Fig. 3(c-g) and (q-s)): up to  $T/T_c \sim 0.7$  the data points from the overdoped samples [Figs. 3(c,g,s)] correspond to sharper SC peaks and agree better with the theory. Figure 3(n) constitutes an exception from the above trend, but, in this case, a stronger degree of overheating is suspected. The best agreement between the theory and the experiment can be observed in Figs. 3(h-m), in which case the data points were generated by the “conventional” ILT technique (expected to give the best energy resolution). If these data also stand the test of time with respect to the true temperature of the samples, then such an agreement would amount to a striking success of the present model.

The experimental data in Figs. 3 are also fairly consistent with the first line of the rule (1). As far as the second line of that rule is concerned, then Figs. 3(i) and (n) can be cited as supporting the rule. The data points in Figs. 3(c,g,o,s) while corresponding to  $\Delta(0)/T_c < 4$  show trend towards  $\Delta(T_c) \neq 0$ . However this trend is due to the highest temperature points, which originate from poorly characterized SC peaks. The conclusive verification of rule (1) should thus await further experiments. It should also be noted in this context, that the scanning tunneling spectroscopy studies of Bi-2212[18] and Bi-2201[19], which indicated that  $\Delta(T_c) \neq 0$ , were all performed on the samples exhibiting  $\Delta(0)/T_c > 4$ .

In a future study, I plan to test the model predictions for the specific heat experiments, which should be equally sensitive to the densities of both *A*- and *B*-states.

In conclusion, I express cautious optimism that (i) there exists a two-parametric description of the  $\Delta(T)$ -curves in high- $T_c$  cuprates; (ii) there exists a critical ratio  $\Delta(0)/T_c$ , which signifies a transition between two different kinds of SC states, and (iii) the above critical ratio is approximately equal to 4. The quantitative agreement between the experimental data reproduced in Fig. 3(h-m) and the model calculations also appears quite promising.

The author is grateful to V. M. Krasnov, A. Yurgens, N. Miyakawa, M. Suzuki, and V. N. Zavaritsky for valuable discussions.

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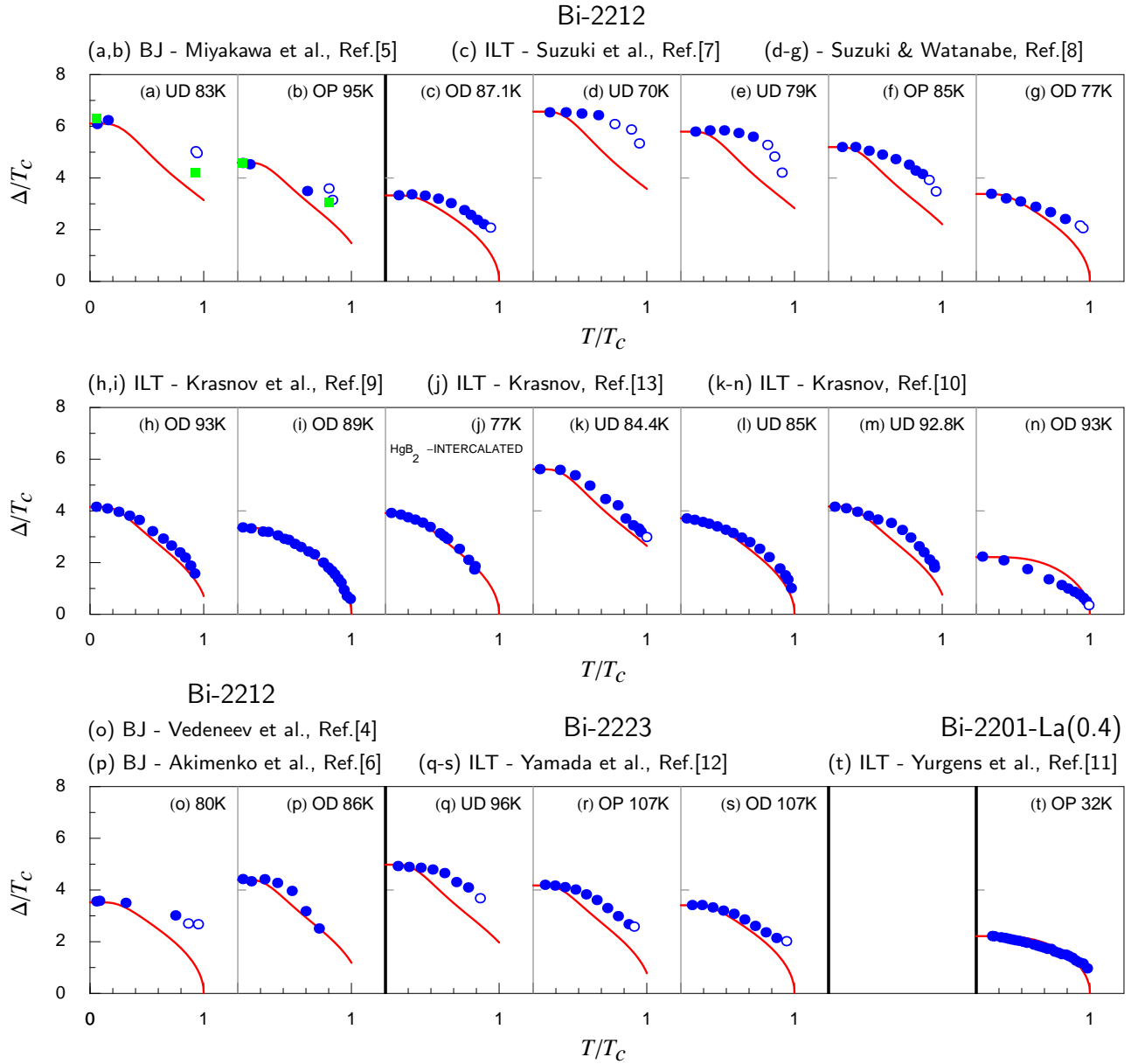


FIG. 3: (Color online) Temperature evolution of the SC gap. Solid lines - theory; circles - experiments; BJ - break junction; ILT - interlayer tunneling. Horizontal marks in each frame indicate  $\Delta/T_c = 4$ . Whenever the original tunneling spectra were reported (a-h, k, n-t), filled circles indicate reasonably well-pronounced SC peaks, while open circles indicate very broad and small SC peaks. Filled circles in frames (i,j,l,m) imply no additional information about the SC peaks. Squares in frames (a,b) represent the “bare” values of  $\Delta$  estimated in Ref.[5].

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